

Your Name _____

Section _____

Names of Collaborators(if any) _____

Chem 226/ Fall 2004

Dr. Rusay

Worksheet (IV)

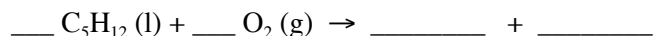
Hydrocarbon Stabilities / Isomerism: Value for your gasoline dollar.

Part I:

Experimental combustion data was obtained for three constitutional (structural) isomers of pentane from the NIST (National Institute of Standards) WebBook which follow. The heat of combustion data lists the lowest and highest values from a series of different reported experimental values.

(1) n-pentane	-3509 to -3536 kJ/mol
(2) 2,2-dimethyl propane	-3490 to -3514 kJ/mol
(3) 2-methylbutane	-3503 to -3528 kJ/mol

A) Complete and balance the chemical equation for the combustion reaction.



Rank the alkanes in order of stability from most stable to least.

___ > ___ > ___

B) Draw an energy diagram that illustrates the combustion data for the three compounds.

$\Delta H_{\text{combustion}}$



C) Briefly explain why the compounds don't produce the same heats of combustion even though they have the same molecular formulas and same number and types of bonds.

D) Determine the one that you would want to burn in your car if they each sold at the same price per gallon. Use \$2.00/gallon as a price. (Note: It is \$ per unit of volume). 1) Calculate the amounts to complete the table. You will need the respective density for each isomer. Two are quite easy to find using *ChemFinder*; the third, 2-methyl butane, is 0.591 g/mL. Circle the most economical selection for your car (1), (2) or (3). 2) Show one calculation for \$ /mol and another for \$/kJ using one of the three constitutional isomers as an example. (Can attach on a separate sheet if necessary.)

	\$ /mol	\$ / kJ
(1)		
(2)		
(3)		

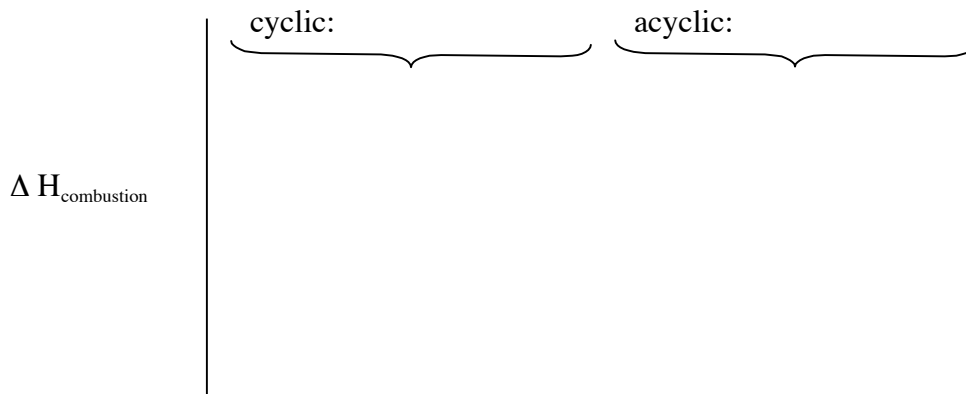
Part II:

Search the NIST database (WebBook) that can be accessed through the course Web resources page . You should find 14 structures. (Two are redundant! So there are actually twelve different constitutional or geometric isomers (E,Z or cis,trans)). The last two #13 & #14 can be ignored.

A) Organize the 12 compounds into two groups: an **acyclic group** (6) and a **cyclic group** (6). Enter line structures for each in the table below; beginning with the largest ring structure for the cyclic and the least substituted for the acyclic. Add the respective combustion data for each compound to the table using data for combustion of liquids (the condensed form) from the NIST WebBook.

Cyclic	Line Drawing	$\Delta H_{\text{combustion}}$	Acyclic	Line Drawing	$\Delta H_{\text{combustion}}$
1			1		
2			2		
3			3		
4			4		
5			5		
6			6		

Draw energy diagrams which illustrates the combustion data for each of the cyclic and acyclic compounds.



B) For the cyclic group rank the compounds in order of stability from highest to lowest.:

_____ > _____ > _____ > _____ > _____ > _____

C) For the acyclic group rank the compounds in order of stability from highest to lowest.:

_____ > _____ > _____ > _____ > _____ > _____

D) Analyze the data looking for patterns and trends. Explain any trends and what structural features could contribute to differences between the structures of the isomers and the energy produced from burning each of them.

E) From the data are cis or trans isomers more stable? Briefly explain why from a molecular basis.

F) From the data are larger rings more or less stable? Briefly explain why from a molecular basis.

Part III:

Are more stable or less stable hydrocarbons better economically as automobile fuels? Explain why by referring to specific examples from the series of compounds you examined.

Bonus Questions:

(If you answer these, include them on a separate sheet and attach it.)

2-methylbutene produces 2-methylbutane on hydrogenation. 111.6 kJ are given off per mole of 2-methylbutene. Isomerization of n-pentane produces 2-methylbutane. The heat of reaction is - 7.78 kJ/mol.

1) What is the energy difference in the stabilities of n-pentane and 2-methylbutane? Provide a value for the stability difference in kJ relative to the more stable isomer.

Double bonds in common ring systems are almost always cis, eg. cyclohexene. However, in cyclooctene, trans-cyclooctene is possible as well as cis-cyclooctene.

2) Explain what could possibly account for this apparent anomaly.

3) Which would theoretically be expected to provide more energy from burning cis-1,2-dimethylcyclopropane or trans-1,2-dimethylcyclopropane? Briefly explain your answer and if the difference is significant.